

Study points to new means of overcoming antiviral resistance in influenza

July 12 2011

UC Irvine researchers have found a new approach to the creation of customized therapies for virulent flu strains that resist current antiviral drugs.

Using powerful [computer simulations](#), UCI's Rommie Amaro and Robin Bush created a method to predict how pocket structures on the surface of influenza proteins promoting [viral replication](#) can be identified as these proteins evolve, allowing for possible pharmaceutical exploitation.

"Our results can influence the development of new drugs taking advantage of this unique feature," said Amaro, assistant professor of pharmaceutical sciences and computer science. The study appears online in *Nature Communications*.

The search for effective [flu drugs](#) has always been hampered by the [influenza virus](#) itself, which mutates from strain to strain, making it difficult to target with a specific pharmaceutical approach.

The most common clinical flu treatments are broad-based and only partially effective. They work by interrupting the action of an [enzyme protein](#) in the virus called neuraminidase, which plays a critical role in viral replication.

In 2006, scientists discovered that avian influenza neuraminidase exhibited a distinctive, pocket-shaped feature in the area pinpointed by clinically used drugs. They named it the 150-cavity.

Amaro and Bush, associate professor of ecology & evolutionary biology, conducted research at the San Diego Supercomputer Center and the National Institute for Computational Sciences to learn the conditions under which the pockets form.

They created molecular simulations of flu proteins to predict how these dynamic structures move and change and where and when the 150-cavity pockets will appear on the protein surface. This sequence analysis method could be utilized on evolving [flu strains](#), providing vital information for drug design, Amaro said.

She added: "Having additional antivirals in our treatment arsenal would be advantageous and potentially critical if a highly virulent strain – for example, H5N1 – evolved to undergo rapid transmission among humans or if the already highly transmissible H1N1 pandemic virus was to develop resistance to existing antiviral drugs."

Provided by University of California - Irvine

Citation: Study points to new means of overcoming antiviral resistance in influenza (2011, July 12) retrieved 24 April 2024 from <https://medicalxpress.com/news/2011-07-antiviral-resistance-influenza.html>

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